Benzamide, 4-bromo-N-ethyl-N-methyl-

Inchi: InChI=1S/C10H12BrNO/c1-3-12(2)10(13)8-4-6-9(11)7-5-8/h4-7H,3H2,1-2H3
InchiKey: SVPOAFUQJSDMQW-UHFFFAOYSA-N
Formula: C10H12BrNO
SMILES: CCN(C)C(=O)c1ccc(Br)cc1
Mol. weight [g/mol]: 242.11

Physical Properties

Property code	Value	Unit	Source
gf	132.28	kJ/mol	Joback Method
hf	-43.39	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	56.02	kJ/mol	Joback Method
log10ws	-3.20		Crippen Method
logp	2.541		Crippen Method
mcvol	157.050	ml/mol	McGowan Method
pc	3333.53	kPa	Joback Method
rinpol	1953.00		NIST Webbook
rinpol	1953.00		NIST Webbook
tb	592.33	K	Joback Method
tc	818.94	K	Joback Method
tf	383.60	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.06	J/mol×K	592.33	Joback Method
cpg	362.17	J/mol×K	630.10	Joback Method
cpg	374.34	J/mol×K	667.87	Joback Method
cpg	385.63	J/mol×K	705.63	Joback Method
cpg	396.10	J/mol×K	743.40	Joback Method
cpg	405.81	J/mol×K	781.17	Joback Method
cpg	414.81	J/mol×K	818.94	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415448&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume